Comment on "Excitons in Molecular Aggregates with Levy-Type Disorder

Eisfeld, A.; Vlaming, S. M.; Moebius, S.; Malyshev, V.A.; Knoester, J.

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Eisfeld *et al.* Reply: The authors of the preceding Comment [1] questioned our statement regarding the unconventional disorder scalings of the HWHM and the nonuniversality of the localization length (LL) distribution reported by us our Letter [2]. We attributed these findings to originate from segmentation caused by the occurrence of outliers [2]. We demonstrate here that our conclusions are correct and that the criticism in Ref. [1] is a consequence of focusing on small values of the disorder strength σ.

The conventional σ scaling for the HWHM (derived in Ref. [2] for linear chains with site disorder drawn from general symmetric α-stable distributions) reads HWHM $\sim J(\sigma/J)^{2\alpha/(1+\alpha)}$, J being the intersite nearest neighbor interaction. Here, segmentation is not taken into account. Outliers become more abundant for smaller α. By equating N^* and $\bar{N}_{\rm seg}$ from Eqs. (3) and (4) in Ref. [2], one can estimate the value of σ above which segmentation starts to play a role [see shaded region in Fig. 1(a)].

For $\sigma \lesssim J$ (values of interest for many molecular systems), deviations from the conventional HWHM σ scaling are not seen for $\alpha = 2$ and 1 (Gaussian and Lorentzian disorder, respectively). However, for $\alpha \lesssim 0.5$, we found clear deviations.

This is shown in Figs. 1(b) and 1(c), where for $\sigma \gtrsim 0.4$ the conventional scaling (solid red lines) clearly breaks down. Moreover, the data points show kinks at which the HWHM suddenly jumps. This is not noise. It can be attributed to structure in the high-energy wing of the absorption spectrum, which grows upon increasing σ, as a consequence of segmentation [2]. Both effects become more pronounced for smaller α. The data also show that these features cannot be adequately fitted by a power law. Finally, we point out that the straight reference line in Fig. 2 of Ref. [2] is irrelevant and has no effect on the conclusion of the existence of exchange broadening of the absorption spectrum.

Next, we demonstrate the nonuniversality of the LL distribution due to segmentation by outliers. Figure 2 displays the normalized LL distributions obtained for $\alpha = 0.5$ using the same scaling of the energy interval as in Refs. [1,3]. In Fig. 2(a), small $\sigma \leq 0.1J$ are considered, as in Ref. [1]. Segmentation is irrelevant here and the normalized LL distributions are nearly identical. Yet, already for $\sigma = 0.1J$, deviations become visible in the appearance of sharp peaks at small LL. Upon increasing σ [Fig. 2(b)], the deviations become more pronounced, and the nonuniversal character of the LL distribution is clear. This is the effect of outliers. In Ref. [1] it is stated that the conventional scalings break down at high σ values, only because $N_{\rm loc}$ approaches unity: a trivial effect. We have demonstrated that the breakdown of scalings found by us is more subtle and is related to a frequent occurrence of outliers when $\alpha \lesssim 0.5$.

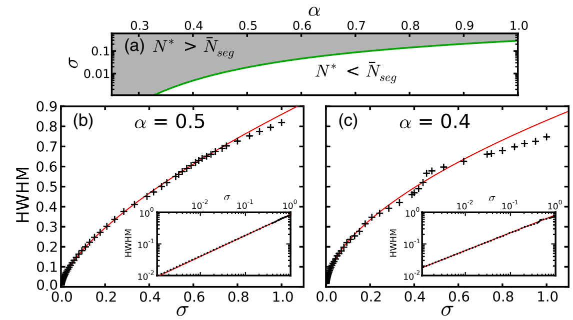

FIG. 1 (color online). (a) Diagram showing for which (α, σ) the chain segmentation dominates localization (shaded area). (b), (c) HWHM σ scaling of the absorption peak. Data (+), results of numerical simulations ($N = 200$); red curves, conventional scaling law.

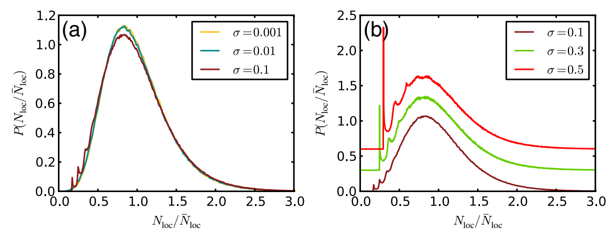

FIG. 2 (color online). Normalized LL distributions calculated for $\alpha = 0.5$ ($N = 200$). In (b), the curves have different vertical offsets to better show their distinction.

A. Eisfeld,[1] S. M. Vlaming,[2,3] S. Möbius,[1]
V. A. Malyshev,[2] and J. Knoester[2]
[1]Max Planck Institute for Physics of Complex Systems
Nöthnitzer Strasse 38, D-01187 Dresden, Germany
[2]Centre for Theoretical Physics
and Zernike Institute for Advanced Materials
University of Groningen
Nijenborgh 4, 9747 AG Groningen, The Netherlands
[3]Department of Chemistry
Massachusetts Institute of Technology
77 Massachusetts Avenue
Cambridge, Massachusetts 02139, USA

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